August 4, 2000

SUBJECT: REQUEST FOR QUOTATION (RFQ) 53SBNB067067

REFERENCE: MASS SPECTRA ASSESSMENT SERVICES

TO: ALL PROSPECTIVE OFFERORS

You are invited to submit a quote to the National Institute of Standards and Technology (NIST) to provide Mass Spectra Assessment Services.

The designated Standard Industrial Code (SIC) for this procurement is 8748 and the related small business size standard if \$5 million. This requirement is 100% Small Business Set aside.

FAR Clause 52.213-4 Terms and Conditions-Simplified Acquisitions (Other than Commercial Items (July 2000) applies to this acquisition.

Department of Commerce Agency-Level Protest Procedures Level Above the Contracting Officer (DEC 1996) applies to this acquisition. The full text of this clause may be accessed electronically at this address: http://www.nist/gov/admin/od/contract/protest.htm

Quotations are to be received at the address not later than 3:00 P.M. local time on August 18, 2000.

National Institute of Standards and Technology Acquisition and Assistance Division Building 301, Room B117 100 Bureau Drive, STOP 3572 Gaithersburg, MD 20899-3572

All questions regarding this solicitation are to be submitted to Diane Loeb, Contracting Officer, on (301) 975-6399, via email <u>dloeb@nist.gov</u> no later than August 11, 2000

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28. CONTRACTOR IS REQUIRED TO SIGN THIS DOCUMENT AND RETURN  3 COPIES TO ISSUING OFFICE. CONTRACTOR AGREES TO    YOUR OFFER ON SOLICITATION   Contract   C												
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# ORDER FOR SUPPLIES AND SERVICES SCHEDULE - CONTINUATION

PAGE NO.

2

IMPORTANT: Mark all packages and papers with contract and/or order numbers.

DATE OF ORDER CONTRACT NO. ORDER NO. QUANTITY ORDERED (21) QUANTI! ACCEPTI ITEM NO. (19) SUPPLIES OR SERVICES (20) UNIT (22) UNIT PRICE **AMOUNT** (23) (24) MASS SPECTRA USING THE STRUCTURE OF THE COMPOUND AND KNOWN GOOD QUALITY SPECTRA OF SIMILAR COMPOUNDS 0003 OPTION YEAR TWO 8500 EA. ASSESSMENT OF QUALITY OF REPORTED MASS SPECTRA USING THE STRUCTURE 8000 EA. OF THE COMPOUND AND KNOWN GOOD QUALITY SPECTRA OF SIMILAR COMPOUNDS

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#### 1. STATEMENT OF WORK

#### **Background**

Mass spectral assessment services are sought for the Physical and Chemical Properties Division (PCPD) of the Chemical Science and Technology Laboratory of the National Institute of Standards and Technology (NIST). The PCPD has determined that a small number of errors are present in the NIST Mass Spectral Database. This error level is sufficient to decrease the quality of the Database. To reduce this error rate it is necessary to reassess the spectral data already contained in the NIST Mass Spectral Database.

#### Scope of Work

Assessment of the quality of reported mass spectra using the structure of the compound and known good quality spectra of similar compounds.

A high quality mass spectrum must satisfy either or both of the following conditions.

- 1. The mass spectrum of a compound with a given structure is reasonable by using probable losses from the molecular ion.
- 2. The mass spectrum of a compound with a given structure is reasonable given well established rearrangements of ions with corresponding neutral losses from the structure of the presumed starting compound.

A high quality mass spectrum will not exhibit any of the following conditions.

- 3. Contamination by air.
- 4. Contamination by water.
- 5. Contamination by isomers or other species that may coelute in gas chromatography columns.
- 6. Evidence of thermal decomposition of the molecule in the ion source of the mass spectrometer.
- 7. Evidence of ions resulting from species that have no stable ions.

The Database shall be reassessed with each spectra evaluated as follows:

- **A.** The spectrum is a good quality spectrum and should be included as is in the NIST Mass Spectral Database. This spectrum can be explained by conditions 1 and 2.
- **B**. The spectrum contains large contaminant peaks at the low masses, is missing low abundance ions, is missing isotopic ions, or is contaminated to a small extent throughout the mass range. These spectra can be explained by conditions 1 and 2 for the most part. Some portion of the mass spectrum may be due to either condition 3, condition 4, or condition 5 at low levels. The

recommended action must be specified (e.g., delete contaminant peaks, delete low mass peaks, adjust abundances of specific ions, leave spectrum as is but move to replicate library).

- C. The spectrum is low quality. Spectra in this class have been contaminated more seriously, or more peaks have been missed than spectra classified by a B grade. Any spectrum exhibiting a combination of conditions 3, 4 and/or 5 must receive a C grade (e.g. air contamination and isomer contamination). Any spectrum exhibiting large isomer contamination, thermal degradation or signal from unstable ions(conditions 5, 6, and 7) must be given a C grade. The recommended action must be specified as for a grade B spectrum.
- **W.** The spectrum is incorrect. Conditions 1 and 2 are not satisfied. If the error is due to an incorrect chemical structure or chemical name, the contractor shall recommend changes in the chemical structure, chemical name, or chemical formula. The contractor shall recommend whether the spectrum should be deleted from the NIST Mass Spectral Database.

In addition to the information required above, all reassessments shall be identified by at least two identifiers, i.e. NIST #, CAS registry number, or chemical structure. Since the majority of this data is free from errors, it is anticipated that this reassessment will be significantly faster than the initial assessment.

It is anticipated that the contractor will from time to time need direct contact with personnel at NIST to discuss error trends discovered in the data as well as to clarify problems that may be better addressed in a collegial setting. This contact requirement will be deemed satisfactory by regular email communications with NIST personnel. The contractor shall be responsible for providing the proper computer equipment for the programs supplied by NIST (Windows operating system on a PC computer with minimum of 120 Mbytes of free hard disk space).

#### 2. CONTRACTOR 'S QUALIFICATION

The correlation of mass spectra to initial chemical structure cannot be done using computer tools today. It requires a good deal of experience in examining good and bad spectra. The minimum requirements for the bidder are a degree in chemistry and at least two years of experience analyzing mass spectra data for the purpose of finding errors and confirming structure/spectral consistency. Experience with routine mass spectra analysis is not sufficient for this purpose. Published papers showing research in correlating spectra to structure or documented prior experience with such correlations must be provided. The bidder must have demonstrated the ability to evaluate large quantities of Mass Spectral data finding errors due to common mistakes such as saturation, column degradation, compound misidentification or Transcription. This ability must be demonstrated by evidence of large mass spectral evaluations in the public literature or commercial databases that are available for examination at NIST.

#### 3. GOVERNMENT'S RESPONSIBITILITY

NIST will provide to the contractor copies of the spectra to be evaluated along with the names and chemical structures of the presumed starting compounds. These will be provided in the form of electronic files. In order to read the electronic files a copy of the NIST/EPA/NIH Mass Spectrometry Database will be made available to the contractor.

#### 4. DELIVERABLES

For each spectrum the contractor shall grade the quality of the spectrum as A, B, C or W and detail any recommended action.

NIST will provide 16500 mass spectra per year for assessment. NIST will deliver a minimum of 4000 spectra per quarter for assessment. The contractor shall deliver the assessments in the form described above no later than 120 calendar days following the receipt of the spectra and structures from NIST.

#### 5. PERIOD OF PERFORMANCE:

The period of performance shall begin on the effective date of the contract and end no more than fifteen months after the effective date. Two additional option years have been included. These will extend the contract by 12 months for each option year.

#### 6. INVOICING

The contractor may bill NIST on a monthly basis for the analyzed spectra. Invoices shall be submitted in an original and two copies to the following address:

National Institute of Standards and Technology Accounts Payable Office 100 Bureau Drive, MS 3733 Gaithersburg, Md 20899-3733

To constitute a proper invoice for payment include the following information or attached documentation.

#### 7. KEY PERSONNEL

- (a) The Contractor shall assign to this contract the following key personnel:
- (b) During the first ninety (90) days of performance, the Contractor shall make no Substitutions of key personnel unless the substitution is necessitated by illness, death, or termination of employment. The Contractor shall notify the Contracting Officer within 15 calendar days after the occurrence of any of these events and provide the information required by paragraph (c) below. After the initial 90-day period, the Contractor shall submit the information required by paragraph (c) to the Contracting Officer at least 15 days prior to making any permanent substitutions.
- (c) The Contractor shall provide a detailed explanation of the circumstances necessitating the proposed substitutions, complete resumes for the proposed substitutes, and any additional information requested by he Contracting Officer. Proposed substitutions should have comparable qualifications to those of the persons being replaced. The

Contracting Officer will notify the Contractor with 15 calendar days after receipt of all required information of the decision on substitutions. The contract will be modified to reflect any approved changes of key personnel.

#### 8. CONTRACTING OFFICER'S AUTHORITY

The Contracting Officer (CO) is the only person authorized to make or approve any changes in any of the requirements of this purchase order and notwithstanding any provisions contained elsewhere in this purchase order, the said authority remains solely in the CO. In the event that the Contractor makes any changes at the direction of any person other than the CO, the changes will be considered to have been without authority an no adjustment will be made in the purchase order prices to cover any increase in costs incurred as s result thereof.

#### 9. **52.217-8 OPTION TO EXTEND SERVICES (AUG 1989)**

The Government may require continued performance of any services within the limits and at the rates specified in the contract. These rates may be adjusted only as a result of revisions to prevailing labor rates provided by the Secretary of Labor. The option provision may be exercised more than once, but the total extension of performance hereunder shall not exceed 6 months. The Contracting Officer may exercise the option by written notice to the Contractor within the period specified in the Schedule.

#### 10. 52.217-9 OPTION TO EXTEND THE TERM OF THE CONTRACT (MAR 1989)

- (a) The Government may extend the term of this contract by written notice to the Contractor within 60 days prior to the expiration of the contract; provided, that the Government shall give the Contractor a preliminary written notice of its intent to extend at least 60 days before the contract expires. The preliminary notice does not commit the Government to an extension.
- (b) If the Government exercises this option, the extended contract shall be considered to include this option provision.
- (c) The total duration of this contract, including the exercise of any options under this clause, shall not exceed three years.

#### 11. INSTRUCTIONS TO OFFERS

Submission of quotes. Submit signed and dated quotes to the office specified in this solicitation at or before the exact time specified in this solicitation. Offers may be submitted on the SF 1449, letterhead stationery, or as otherwise specified in the solicitation. As a minimum, offers must show—

- (1) The solicitation number;
- (2) The name, address, and telephone number of the offeror;
- (3) Price and any discount terms;
- (4) 'Remit to' address, if different than mailing address;
- (5) A completed copy of the representations and certifications;
- (6) Qualifications offer to provide resume and a list of pertinent publications required in paragraph 2 entitled, "Contractor's Qualifications" above.
- (7) If the offer is not submitted on the SF 1449, include a statement specifying the extent of agreement with all terms, conditions, provisions included in the solicitation. Offers that fail to furnish required representations or information, or reject the terms and conditions of the solicitation may be excluded from consideration.
- (8) Data Universal Numbering System (DUNS) Number. The offer shall enter, in the block with its name and address on the cover page of it's offer, the annotation 'DUNS' followed by the DUNS number that identifies the offeror's name and address. If the offer does not have a DUNS number, it should contact Dun and Bradstreet to obtain one at no charge. An offeror with in the United States may call 1-800-333-0505. The offeror may obtain more information regarding the DUNS number, including locations of local Dun and Bradstreet Information Services offices for offerors located outside the United States, from the Internet home page at http://www.customerservice@dnb.com. If an offeror is unable to locate a local service center, it may send an e-mail to Dun and Bradstreet at globalinfo@mail.dnb.com

#### 12. BASIS OF AWARD

Award will be made to the vendor whose overall quote demonstrates the best value to the Government, price and other factors considered. FAR 52.217-5, Evaluation of Options is applicable.

#### 13. OFFEROR REPRESENTATIONS AND CERTIFICATIONS (JUN 1996)

(a) Definitions.

"Emerging small business" means a small business concern whose size is no greater than 50 percent of the numerical size standard for the standard industrial classification code designated.

"Small business concern" means a concern, including its affiliates, that is independently owned and operated, not dominant in the field of operation in which it is bidding on Government contracts, and qualified as a small business under the criteria in 13 CFR Part 121 and size standards in this solicitation.

"Small disadvantaged business concern" means a small business concern that-

- (1) Is at least 51 percent unconditionally owned by one or more individuals who are both socially and economically disadvantaged, or a publicly owned business, having at least 51 percent of its stock unconditionally owned by one or more socially and economically disadvantaged individuals, and
- (2) Has its management and daily business controlled by one or more such individuals. This term also means a small business concern that is at least 51 percent unconditionally owned by an economically disadvantaged Indian tribe or Native Hawaiian organization, or a publicly owned business having at least 51 percent of its stock unconditionally owned by one or more of these entities, which has its management and daily business controlled by members of an economically disadvantaged Indian tribe or Native Hawaiian organization and which meets the requirements of 13 CFR Part 124.

"Women-owned small business concern" means a small business concern-

(1) Which is at least 51 percent owned by one or more women or, in the case of any publicly owned business, at least 51 percent of the stock of which is owned by one or more women; and

Whose management and daily business operations are controlled by one or more women.

"Women-owned business concern" means a concern which is at least 51 percent owned by one or more women; or in the case of any publicly owned business, at least 51 percent of the stock of which is owned by one or more women; and whose management and daily business operations are controlled by one or more women.

Other. State basis.

(2) Corporate Status.
Corporation providing medical and health care services, or engaged in the billing and collecting of payments for such services;
Other corporate entity;
Not a corporate entity:
Sole proprietorship
Partnership
Hospital or extended care facility described in 26 CFR 501(c)(3) that is exempt from taxation under 26 CFR 501(a).
(3) Common Parent.
Offeror is not owned or controlled by a common parent:
Name and TIN of common parent:
Name
TIN
(c) Offerors must complete the following representations when the resulting contract is to be performed inside the United States, its territories or possessions, Puerto Rico, the Trust Territory of the Pacific Islands, or the District of Columbia. Check all that apply.
(1) Small business concern. The offeror represents as part of its offer that it is, is not a small business concern.
(2) Small disadvantaged business concern. The offeror represents and certifies that it is, is not a small disadvantaged business concern.
(3) Women-owned small business concern. The offeror represents that it is, is not a women-owned small business concern.
Note: Complete paragraphs (c)(4) and (c)(5) only if this solicitation is expected to excee the simplified acquisition threshold.
(4) Women-owned business concern. The offeror represents that it is, is not, women-owned business concern.
(5) Tie bid priority for labor surplus area concerns. If this is an invitation for bid, small business offerors may identify the labor surplus areas in which costs to be

incurred on account of manufacturing or subcontractors) amount to more than 50	* · ·				
and for the Targeted Industry Categorie	usiness Competitiveness Demonstration Program s under the Small Business Competitiveness y if the offeror has certified itself to be a small ds for this solicitation.]				
· · · · · · · · · · · · · · · · · · ·	one of the four designated industry groups				
The offeror represents as part of small business.	its offer that it is, is not an emerging				
· / · •	(ii) (Complete only for solicitations indicated in an addendum as being for one of the targeted industry categories (TICs) or four designated industry groups (DIGs).)				
Offeror represents and certifies a	Offeror represents and certifies as follows:				
Employees column if size	(A) Offeror's number of employees for the past 12 months (check the Employees column if size standard stated in the solicitation is expressed in terms of number of employees); or				
(check the Average Annu	nual gross revenue for the last 3 fiscal years all Gross Number of Revenues column if size icitation is expressed in terms of annual receipts).				
(Check one of the follow	ing):				
Number of Employees	Average Annual Gross Revenues				
50 or fewer 51 - 100 101 - 250 251 - 500 501 - 750 751 - 1,000 Over 1,000	\$1 million or less \$1,000,001 - \$2 million \$2,000,001 - \$3.5 million \$3,500,001 - \$5 million \$5,000,001 - \$10 million \$10,000,001 - \$17 million Over \$17 million				

- (d) Certifications and representations required to implement provisions of Executive Order 11246--
  - (1) Certification of non-segregated facilities. (Applies only if the contract amount is

expected to exceed \$10,000)--

By submission of this offer, the offeror certifies that it does not and will not maintain or provide for its employees, any facilities that are segregated on the basis of race, color, religion, or national origin because of habit, local custom, or otherwise and that it does not and will not permit its employees to perform their services at any location where segregated facilities are maintained. The offeror agrees that a breach of this certification is a violation of the Equal Opportunity clause in the contract.

- (e) Certification Regarding Payments to Influence Federal Transactions (31 U.S.C. 1352). Applies only if the contract is expected to exceed \$100,000.) By submission of its offer, the offeror certifies to the best of its knowledge and belief that no Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress or an employee of a Member of Congress on his or her behalf in connection with the award of any resultant contract.
- (f) Buy American Act-Trade Agreements-Balance of Payments Program Certificate. (Applies only if FAR clause 52.225-9, Buy American Act-Trade Agreement-Balance of Payments Program, is included in this solicitation.) (1) The offeror hereby certifies that each end product, except those listed in paragraph f(2) of this provision, is a domestic end product (as defined in the clause entitled "Buy American Act--Trade Agreements--Balance of Payments Program") and that components of unknown origin have been considered to have been mined, produced, or manufactured outside the United States, a designated country, a North American Free Trade Agreement (NAFTA) country, or a Caribbean Basin country, as defined in section 25.401 of the Federal Acquisition Regulation.
  - (2) Excluded End Products:

COUNTRY OF ORIGIN

(List as necessary)
(3) Offers will be evaluated by giving certain preferences to domestic end products, designated country end products, NAFTA country end products, and Caribbean Basin country end products over other end products. In order to obtain these preferences in the
evaluation of each excluded end product listed in paragraph (f)(2) of this provision, offerors must identify and certify below those excluded end products that are designated or NAFTA country end products, or Caribbean Basin country end products. Products that are not identified and certified below will not be deemed designated country end products, NAFTA country end products, or Caribbean Basin country end products.
Offerors must certify by inserting the applicable line item numbers in the following:
(i) The offeror certifies that the following supplies qualify as "designated or NAFTA country end products" as those terms are defined in the clause entitled "Buy American ActTrade AgreementsBalance of Payments Program":
(Insert line item numbers)
(ii) The offeror certifies that the following supplies qualify as "Caribbean Basin country end products" as that term is defined in the clause entitled "Buy American ActTrade AgreementsBalance of Payments Program":
(Insert line item numbers)
(4) Offers will be evaluated in accordance with FAR Part 25.

LINE ITEM NO.

(g)(1) Buy American Act--North American Free Trade Agreement Implementation Act--Balance of Payments Program. (Applies only if FAR clause 52.225-21, Buy American Act--North American Free Trade Agreement Implementation Act--Balance of Payments Program, is included in this solicitation.) (i) Each end product being offered, except those listed in paragraph (g)(1)(ii) of this provision, is a domestic end product (as defined in the clause entitled "Buy

American Act--North American Free Trade Agreement Implementation Act--Balance of Payments Program." Components of unknown origin have been considered to have been mined, produced, or manufactured outside the United States.

(ii) Excluded End Products:	
LINE ITEM NO.	COUNTRY OF ORIGIN
(List as necessary)	
products or NAFTA country end pro- obtain these preferences in the evalu- paragraph (g)(1)(ii) of this provision end products that are NAFTA country identified below will not be deemed supplies qualify as "NAFTA country	ng certain preferences to domestic end oducts over other end products. In order to ation of each excluded end product listed in a, offerors must identify below those excluded ry end products. Products that are not NAFTA country end products. The following end products" as that term is defined in the North American Free Trade Agreement rements Program"
(Insert line item numbers)	
()	

- (iv) Offers will be evaluated in accordance with Part 25 of the Federal Acquisition Regulation. In addition, if this solicitation is for supplies for use outside the United States, an evaluation factor of 50 percent will be applied to offers of end products that are not domestic or NAFTA country end products.
- (2) Alternate I. If Alternate I to the clause at 52.225-21 is included in this solicitation, substitute the following paragraph (g)(1)(iii) for paragraph (g)(1)(iii) of this provision:
- (g)(1)(iii) Offers will be evaluated by giving certain preferences to domestic end products or Canadian end products over other end products. In order to obtain these preferences in the evaluation of each excluded end product listed in paragraph (b) of this provision, offerors must identify below those excluded end products that are Canadian end products. Products that are not identified below will not be deemed Canadian end products.

The following supplies qualify as "Canadian end products" as that term is defined in the clause entitled "Buy American Act--North American Free Trade Agreement Implementation Act--Balance of Payments Program"

	(Insert line item numbers)
	on Regarding Debarment, Suspension or Ineligibility for Award (Executive Order feror certifies, to the best of its knowledge and belief, that
suspend	e offeror and/or any of its principals are, are not presently debarred, ded, proposed for debarment, or declared ineligible for the award of ets by any Federal agency, and
convict fraud o perforn Federal embezz making not pre	Have, have not, within a three-year period preceding this offer, been sed of or had a civil judgment rendered against them for: commission of or a criminal offense in connection with obtaining, attempting to obtain, or ning a Federal, state or local government contract or subcontract; violation of lor state antitrust statutes relating to the submission of offers; or commission of element, theft, forgery, bribery, falsification or destruction of records, a false statements, tax evasion, or receiving stolen property; and are, are sently indicted for, or otherwise criminally or civilly charged by a Government with, commission of any of these offenses.
	(i) Procurement Integrity Certification (41 U.S.C. 423). (Applies only if the contract is expected to exceed \$100,000.)
	I, the undersigned, am the officer or employee responsible for the preparation of this offer. I certify, to the best of my knowledge and belief, that either
	I have no information, or
	I have disclosed information to the Contracting Officer concerning a violation or possible violation of subsection (a), (b), (d) or (f) of 41 U.S.C. 423, Procurement Integrity, or its implementing regulations that may have occurred during the conduct of this procurement.
	[Signature of the officer or employee responsible for the offer and date]